	ENTRY	SESSION
CA SUBSCRIBER PRICE	-24.74	-24.74

FILE 'REGISTRY' ENTERED AT 19:46:42 ON 21 OCT 2003
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STRUCTURE FILE UPDATES: 20 OCT 2003 HIGHEST RN 607332-91-2
DICTIONARY FILE UPDATES: 20 OCT 2003 HIGHEST RN 607332-91-2

TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2003

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details:
http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf

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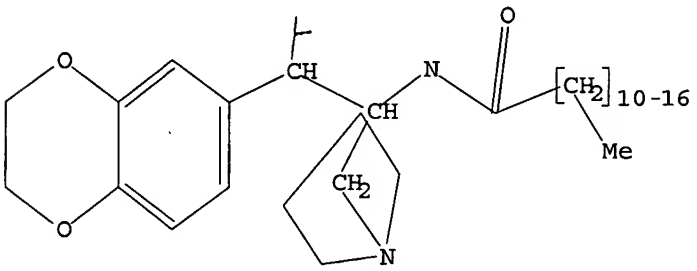
Uploading 030963.str

L8 STRUCTURE UPLOADED

=> d l8
L8 HAS NO ANSWERS
L8 STR



Structure attributes must be viewed using STN Express query preparation.

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SAMPLE SEARCH INITIATED 19:50:18 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 14 TO ITERATE

100.0% PROCESSED 14 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:	ONLINE	**COMPLETE**
	BATCH	**COMPLETE**
PROJECTED ITERATIONS:	56 TO	504
PROJECTED ANSWERS:	0 TO	0

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L9            0 SEA SSS SAM L8

=> s l8 sss full
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100.0% PROCESSED     274 ITERATIONS                                  8 ANSWERS
SEARCH TIME: 00.00.01

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COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                       ENTRY    SESSION
FULL ESTIMATED COST                                   150.15     625.68

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)          SINCE FILE      TOTAL
                                                       ENTRY    SESSION
CA SUBSCRIBER PRICE                                     0.00     -24.74

FILE 'CAPLUS' ENTERED AT 19:50:34 ON 21 OCT 2003
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FILE COVERS 1907 - 21 Oct 2003  VOL 139 ISS 17
FILE LAST UPDATED: 20 Oct 2003  (20031020/ED)

  This file contains CAS Registry Numbers for easy and accurate
  substance identification.


=> s l10
L11           14 L10

=> d l11 1-14 ibib abs hitstr

L11  ANSWER 1 OF 14  CAPLUS  COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER:         2003:434544  CAPLUS
DOCUMENT NUMBER:          139:6863
TITLE:                    Diastereoselective synthesis of UDP-glucose:n-
                          acylsphingosine glucosyltransferase inhibitors
INVENTOR(S):              Hirth, Bradford H.
PATENT ASSIGNEE(S):       Genzyme Corporation, USA
SOURCE:                   PCT Int. Appl., 38 pp.
                          CODEN: PIXXD2
DOCUMENT TYPE:            Patent
LANGUAGE:                 English
FAMILY ACC. NUM. COUNT:   1
PATENT INFORMATION:
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PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003045928	A1	20030605	WO 2002-US38206	20021126

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VC, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

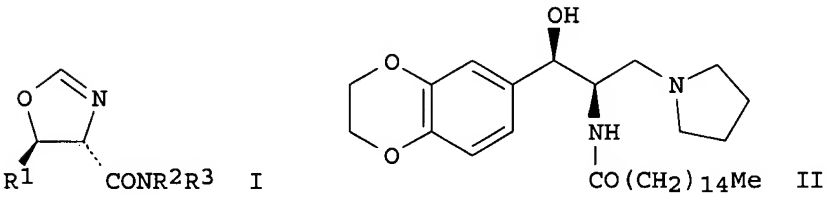
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

US 2003153768	A1	20030814	US 2002-305787	20021126

PRIORITY APPLN. INFO.: US 2001-333392P P 20011126

OTHER SOURCE(S): CASREACT 139:6863; MARPAT 139:6863

GI



AB Oxazolines I [R1 = (un)substituted aryl; R2, R3 = h, (un)substituted aliph.; NR2R3 = heterocyclic] are pred. as intermediates for UDP-glucose:n-acylsphingosine glucosyltransferase inhibitors form R1CHO and R2R3NCOCH2CN. Thus, CNCH2CO2Me was treated with pyrrolidine and the amide was treated with 1,4-benzodioxane-6-carboxaldehyde, followed by hydrolysis of the oxazoline, redn. of the keto group, and acylation with palmitoyl chloride to give the UDP-glucose:n-acylsphingosine glucosyltransferase inhibitor II.

IT **245329-83-3P**

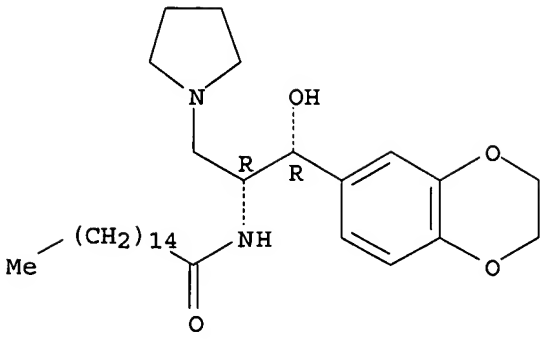
RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(stereoselective synthesis of UDP-glucose:n-acylsphingosine glucosyltransferase inhibitors)

RN 245329-83-3 CAPLUS

CN Hexadecanamide, N-[(1R,2R)-2-(2,3-dihydro-1,4-benzodioxin-6-yl)-2-hydroxy-1-(1-pyrrolidinylmethyl)ethyl]-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



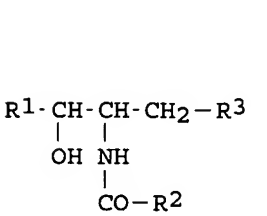
REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 2 OF 14 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 2003:300612 CAPLUS
DOCUMENT NUMBER: 138:321048
TITLE: Preparation of amino ceramide-like compounds as glucosyl ceramide (GlcCer) formation inhibitors
INVENTOR(S): Shayman, James A.; Radin, Norman S.
PATENT ASSIGNEE(S): The Regents of the University of Michigan, USA
SOURCE: U.S. Pat. Appl. Publ., 32 pp., Cont.-in-part of U.S. 870,870.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 4
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2003073680	A1	20030417	US 2002-134315	20020429
US 5916911	A	19990629	US 1996-708574	19960905
US 5945442	A	19990831	US 1997-883217	19970626
US 5952370	A	19990914	US 1997-882772	19970626
US 6040332	A	20000321	US 1997-882773	19970626
US 6030995	A	20000229	US 1998-182161	19981029
US 6255336	B1	20010703	US 1999-350768	19990709
US 2001041735	A1	20011115	US 2001-870870	20010531
US 6569889	B2	20030527		

PRIORITY APPLN. INFO.:
US 1995-4047P P 19950920
US 1996-708574 A3 19960905
US 1997-883218 A2 19970626
US 1999-350768 A3 19990709
US 2001-870870 A2 20010531

OTHER SOURCE(S): MARPAT 138:321048
GI



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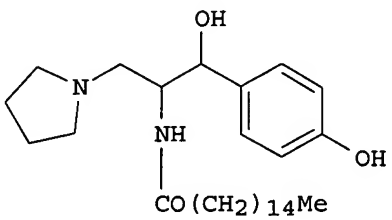

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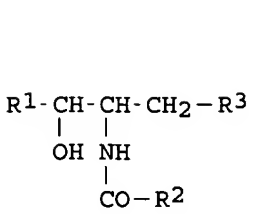

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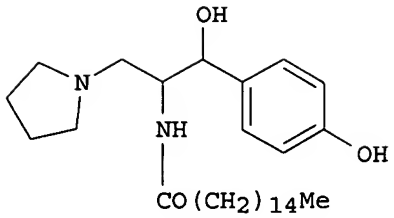


II

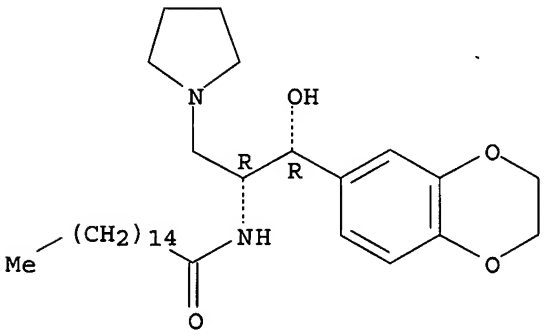
AB The present invention provides amino ceramide-like compds. of formula I [R1 = (substituted) Ph, alkyl, etc.; R2 = fatty acid residue; R3 = tertiary amine] which inhibit glucosyl ceramide (GlcCer) formation by inhibiting the enzyme GlcCer synthase, thereby lowering the level of glycosphingolipids. The compds. of the present invention have improved GlcCer synthase inhibition activity and are therefore useful in therapeutic methods for treating various conditions and diseases assocd. with altered glycosphingolipid levels. Thus, II was prepd. and found to inhibit GlcCer synthesis.

IT **245329-78-6P 511538-27-5P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of amino ceramide-like compds. as glucosylceramide formation inhibitors)

RN 245329-78-6 CAPLUS

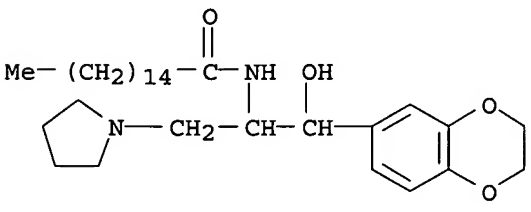
CN Hexadecanamide, N-[(1R,2R)-2-(2,3-dihydro-1,4-benzodioxin-6-yl)-2-hydroxy-1-(1-pyrrolidinylmethyl)ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



RN 511538-27-5 CAPLUS

CN Hexadecanamide, N-[2-(2,3-dihydro-1,4-benzodioxin-6-yl)-2-hydroxy-1-(1-pyrrolidinylmethyl)ethyl]- (9CI) (CA INDEX NAME)

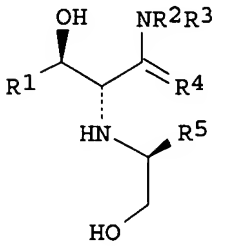


L11 ANSWER 3 OF 14 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 2003:76767 CAPLUS
DOCUMENT NUMBER: 138:137087
TITLE: Preparation of ceramide analogs as UDP-glucose: N-acylsphingosine glucosyltransferase inhibitors and intermediates thereof
INVENTOR(S): Hirth, Bradford H.; Siegel, Craig
PATENT ASSIGNEE(S): Genzyme Corporation, USA
SOURCE: PCT Int. Appl., 71 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003008399	A1	20030130	WO 2002-US22659	20020716
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 2003050299	A1	20030313	US 2002-197227	20020716

PRIORITY APPLN. INFO.: US 2001-305814P P 20010716
OTHER SOURCE(S): MARPAT 138:137087
GI



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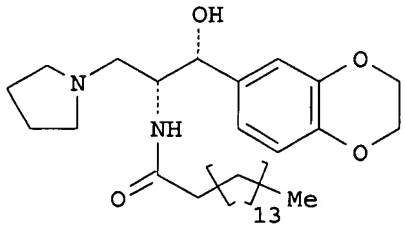


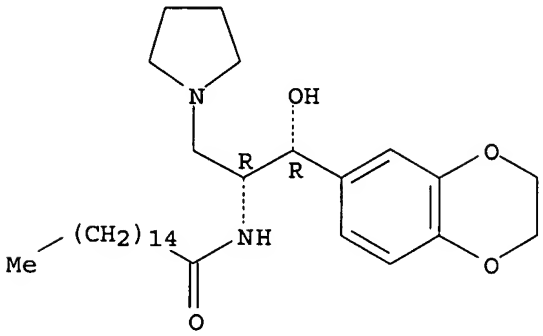
II

AB Ceramide analogs, such as I [R1, R5 = un(substituted) arom.; R2, R3 = H, un(substituted) aliph.; NR2R3 = (un)substituted non-arom. heterocyclic ring; R4 = O, H2], were prepd. for their therapeutic use as UDP-glucose: N-acylsphingosine glucosyltransferase inhibitors (no data). Thus, ceramide analog II was prepd. via a multistep synthetic sequence starting from S-(+)-Ph glycinol, phenyl-.alpha.-bromoacetate, 1,4-benzodioxan-6-carboxaldehyde, pyrrolidine and palmitoyl chloride. Also disclosed are novel intermediates formed during the synthesis of I.

IT **245329-78-6P**
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
(prepn. of ceramide analogs as UDP-glucose: N-acylsphingosine glucosyltransferase inhibitors and intermediates thereof)

RN 245329-78-6 CAPLUS
CN Hexadecanamide, N-[(1R,2R)-2-(2,3-dihydro-1,4-benzodioxin-6-yl)-2-hydroxy-1-(1-pyrrolidinylmethyl)ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 4 OF 14 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 2002:978472 CAPLUS
DOCUMENT NUMBER: 138:39140
TITLE: Preparation of amino ceramide like prodrugs for therapeutic use in the treatment of conditions associated with altered glycosphingolipid levels
INVENTOR(S): Shayman, James A.; Radin, Norman S.
PATENT ASSIGNEE(S): USA
SOURCE: U.S. Pat. Appl. Publ., 13 pp., Cont.-in-part of U.S. Ser. No. 44,869.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2002198240	A1	20021226	US 2002-134314	20020429
US 2002156107	A1	20021024	US 2002-44869	20020110

PRIORITY APPLN. INFO.: US 2001-260948P P 20010110
US 2001-262196P P 20010117
US 2002-44869 A2 20020110
OTHER SOURCE(S): MARPAT 138:39140
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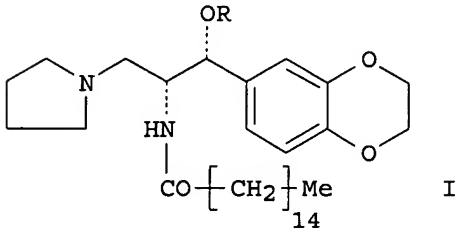


I

AB Novel prodrugs of amino ceramide-like compds., such as R3CH2CH(NHCOR2)CH(R1)OR4 [R1 = arom., alicyclic, or aliph. groups; R2 = (CH2)nMe, n = 2-18; R3 = tertiary amine; R4 = CO(CH2)mMe, dihydropyridiylcarbonyl; m = 0; m .gtoreq. 1], were prepd for pharmaceutical use in the treatment of diseases, such as cancer, microbial

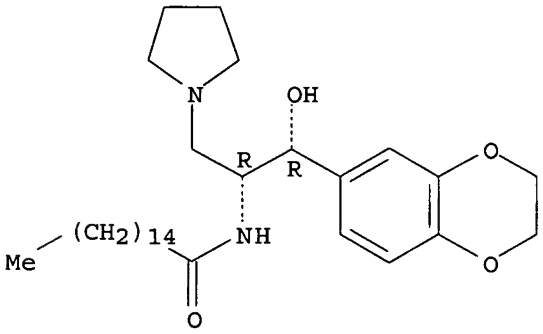
or viral infections, and sphingolipidosis. The compds. of the present invention have improved glucosylceramide synthase (GlcCer) inhibition activity and are therefore highly useful in therapeutic methods for treating various conditions and diseases assocd. with altered glycosphingolipid levels. Thus, acetate I (R = COMe) was prepd. by acetylation of the corresponding alc I (R = H) with acetic anhydride by stirring in pyridine at rt for 2 days.

IT **245329-78-6**
RL: PAC (Pharmacological activity); RCT (Reactant); THU (Therapeutic use); BIOL (Biological study); RACT (Reactant or reagent); USES (Uses)
(prepn. of amino ceramide like prodrugs for therapeutic use in the treatment of conditions assocd. with altered glycosphingolipid levels)

RN 245329-78-6 CAPLUS

CN Hexadecanamide, N-[(1R,2R)-2-(2,3-dihydro-1,4-benzodioxin-6-yl)-2-hydroxy-1-(1-pyrrolidinylmethyl)ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

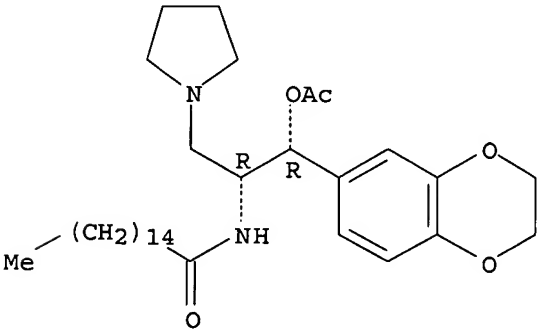


IT **445467-63-0P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of amino ceramide like prodrugs for therapeutic use in the treatment of conditions assocd. with altered glycosphingolipid levels)

RN 445467-63-0 CAPLUS

CN Hexadecanamide, N-[(1R,2R)-2-(acetyloxy)-2-(2,3-dihydro-1,4-benzodioxin-6-yl)-1-(1-pyrrolidinylmethyl)ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



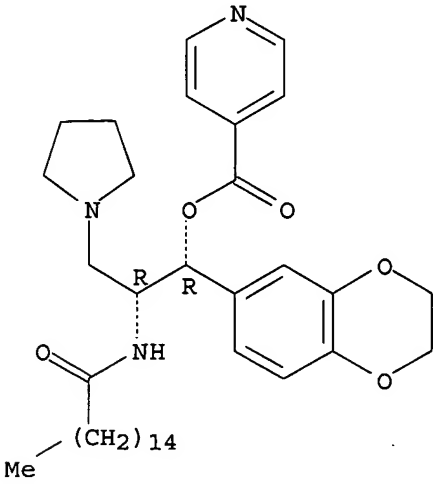
IT **478686-04-3P 478686-05-4DP**, derivs.
RL: PNU (Preparation, unclassified); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of amino ceramide like prodrugs for therapeutic use in the

treatment of conditions assocd. with altered glycosphingolipid levels)

RN 478686-04-3 CAPLUS

CN 4-Pyridinecarboxylic acid, (1R,2R)-1-(2,3-dihydro-1,4-benzodioxin-6-yl)-2-[(1-oxohexadecyl)amino]-3-(1-pyrrolidinyl)propyl ester (9CI) (CA INDEX NAME)

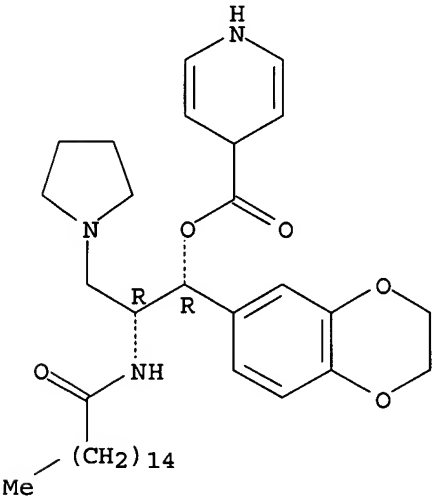
Absolute stereochemistry.



RN 478686-05-4 CAPLUS

CN 4-Pyridinecarboxylic acid, 1,4-dihydro-, (1R,2R)-1-(2,3-dihydro-1,4-benzodioxin-6-yl)-2-[(1-oxohexadecyl)amino]-3-(1-pyrrolidinyl)propyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT **478686-03-2P**

RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

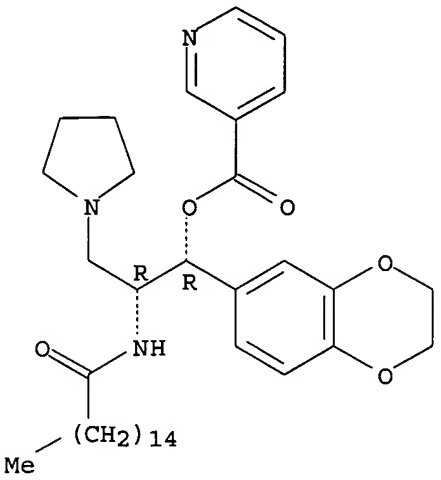
(prepn. of amino ceramide like prodrugs for therapeutic use in the treatment of conditions assocd. with altered glycosphingolipid levels)

RN 478686-03-2 CAPLUS

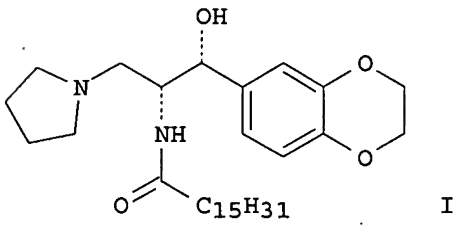
CN 3-Pyridinecarboxylic acid, (1R,2R)-1-(2,3-dihydro-1,4-benzodioxin-6-yl)-2-[(1-oxohexadecyl)amino]-3-(1-pyrrolidinyl)propyl ester (9CI) (CA INDEX

NAME)

Absolute stereochemistry.



L11 ANSWER 5 OF 14 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 2002:808778 CAPLUS
DOCUMENT NUMBER: 138:255175
TITLE: syn-Selective additions to Garner aldehyde: synthesis of a potent glucosylceramide synthase inhibitor
AUTHOR(S): Husain, Arifa; Ganem, Bruce
CORPORATE SOURCE: Baker Laboratory, Department of Chemistry and Chemical Biology, Cornell University, Ithaca, NY, 14853-1301, USA
SOURCE: Tetrahedron Letters (2002), 43(47), 8621-8623
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 138:255175
GI



I

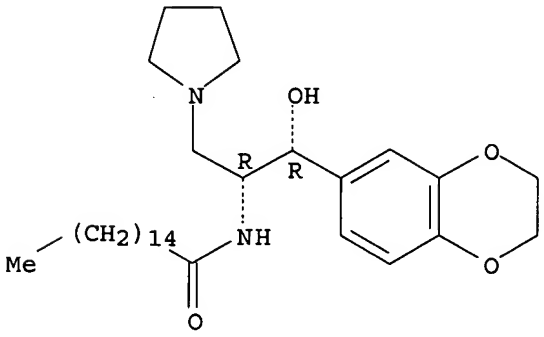
AB Highly syn-selective addns. of aryl Grignard reagents to Garner aldehyde are reported, making possible a practical, asym. synthesis of the potent glucosylceramide synthase inhibitor I.

IT **245329-78-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(syn-selective Grignard addns. to Garner aldehyde and synthesis of a potent glucosylceramide synthase inhibitor)

RN 245329-78-6 CAPLUS
CN Hexadecanamide, N-[(1R,2R)-2-(2,3-dihydro-1,4-benzodioxin-6-yl)-2-hydroxy-

1-(1-pyrrolidinylmethyl)ethyl]- (9CI) (CA INDEX NAME)

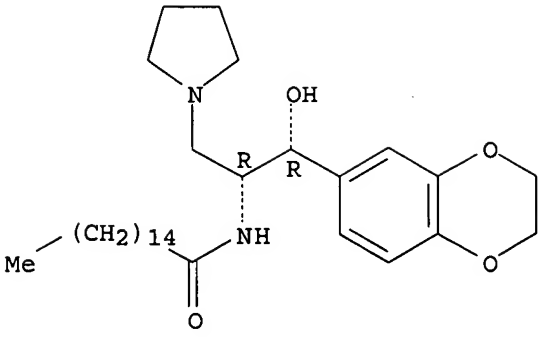
Absolute stereochemistry. Rotation (+).



REFERENCE COUNT: 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 6 OF 14 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 2002:668355 CAPLUS
DOCUMENT NUMBER: 139:257892
TITLE: Disruption of the glucosylceramide biosynthetic pathway in Aspergillus nidulans and Aspergillus fumigatus by inhibitors of UDP-Glc: ceramide glucosyltransferase strongly affects spore germination, cell cycle, and hyphal growth. [Erratum to document cited in CA138:69685]
AUTHOR(S): Levery, Steven B.; Momany, Michelle; Lindsey, Rebecca; Toledo, Marcos S.; Shayman, James A.; Fuller, Matthew; Brooks, Kelly; Doong, Ron Lou; Straus, Anita H.; Takahashi, Helio K.
CORPORATE SOURCE: Department of Chemistry, University of New Hampshire, Durham, NH, 03824, USA
SOURCE: FEBS Letters (2002), 526(1-3), 151
CODEN: FEBLAL; ISSN: 0014-5793
PUBLISHER: Elsevier Science B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB On page 59, Introduction, second paragraph, lines 4-8 should read as follows: "However, despite a no. of studies demonstrating intriguing physiol. activities of exogenously added fungal cerebrosides [11-14], the true in vivo functions of these compds. remain unclear.".
IT **245329-78-6**
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(disruption of glucosylceramide biosynthetic pathway in Aspergillus (Erratum))
RN 245329-78-6 CAPLUS
CN Hexadecanamide, N-[(1R,2R)-2-(2,3-dihydro-1,4-benzodioxin-6-yl)-2-hydroxy-1-(1-pyrrolidinylmethyl)ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



L11 ANSWER 7 OF 14 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 2002:615591 CAPLUS
DOCUMENT NUMBER: 137:150282
TITLE: Amino ceramide-like compounds and therapeutic methods of use
INVENTOR(S): Shayman, James A.; Radin, Norman S.
PATENT ASSIGNEE(S): The Regents of the University of Michigan, USA
SOURCE: PCT Int. Appl., 25 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002062777	A2	20020815	WO 2002-US808	20020110
WO 2002062777	A3	20021128		
WO 2002062777	C2	20030109		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.: US 2001-260948P P 20010110
US 2001-262196P P 20010117

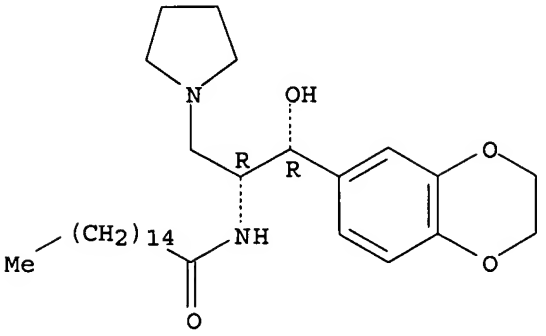
OTHER SOURCE(S): MARPAT 137:150282

AB Novel prodrugs of amino ceramide-like compds. are provided which inhibit glucosyl ceramide (GlcCer) formation by inhibiting the enzyme GlcCer synthase, thereby lowering the level of glycosphingolipids. The compds. of the present invention have improved GlcCer synthase inhibition activity and are therefore highly useful in therapeutic methods for treating various conditions and diseases assocd. with altered glycosphingolipid levels.

IT **245329-78-6**
RL: BSU (Biological study, unclassified); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(prodrugs of amino ceramide-like compds. which inhibit glucosyl ceramide synthase for treatment of diseases assocd. with altered glycosphingolipid levels)

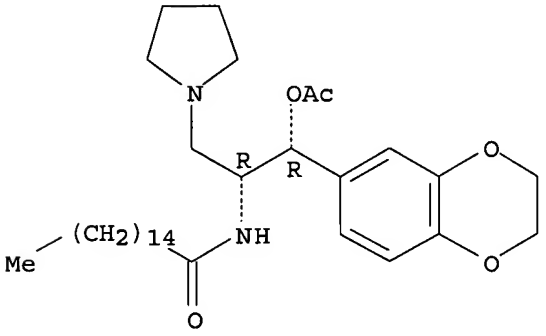
RN 245329-78-6 CAPLUS
CN Hexadecanamide, N-[(1R,2R)-2-(2,3-dihydro-1,4-benzodioxin-6-yl)-2-hydroxy-1-(1-pyrrolidinylmethyl)ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



IT **445467-63-0**
RL: PAC (Pharmacological activity); PKT (Pharmacokinetics); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(prodrugs of amino ceramide-like compds. which inhibit glucosyl ceramide synthase for treatment of diseases assocd. with altered glycosphingolipid levels)
RN 445467-63-0 CAPLUS
CN Hexadecanamide, N-[(1R,2R)-2-(acetyloxy)-2-(2,3-dihydro-1,4-benzodioxin-6-yl)-1-(1-pyrrolidinylmethyl)ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L11 ANSWER 8 OF 14 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 2002:602526 CAPLUS
DOCUMENT NUMBER: 138:69685
TITLE: Disruption of the glucosylceramide biosynthetic pathway in Aspergillus nidulans and Aspergillus fumigatus by inhibitors of UDP-Glc:ceramide glucosyltransferase strongly affects spore germination, cell cycle, and hyphal growth
AUTHOR(S): Levery, Steven B.; Momany, Michelle; Lindsey, Rebecca; Toledo, Marcos S.; Shayman, James A.; Fuller, Matthew; Brooks, Kelly; Doong, Ron Lou; Straus, Anita H.; Takahashi, Helio K.
CORPORATE SOURCE: Department of Chemistry, University of New Hampshire, Durham, NH, 03824, USA
SOURCE: FEBS Letters (2002), 525(1-3), 59-64
CODEN: FEBLAL; ISSN: 0014-5793
PUBLISHER: Elsevier Science B.V.
DOCUMENT TYPE: Journal

LANGUAGE: English

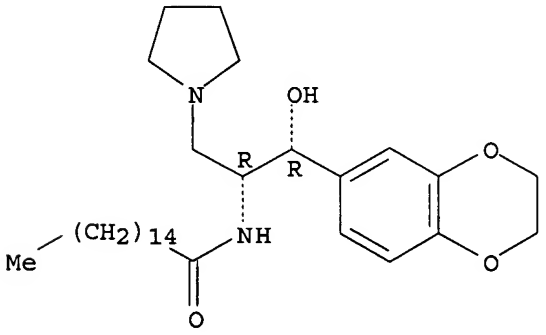
AB The opportunistic mycopathogen Aspergillus fumigatus expresses both glucosylceramide and galactosylceramide (GlcCer and GalCer), but their functional significance in Aspergillus species is unknown. We here identified and characterized a GlcCer from Aspergillus nidulans, a non-pathogenic model fungus. Involvement of GlcCer in fungal development was tested on both species using a family of compds. known to inhibit GlcCer synthase in mammals. Two analogs, D-threo-1-phenyl-2-palmitoylamino-3-pyrrolidinopropanol (P4) and D-threo-3',4'-ethylenedioxy-P4, strongly inhibited germination and hyphal growth. Neutral lipids from A. fumigatus cultured in the presence of these inhibitors displayed a significantly reduced GlcCer/GalCer ratio. These results suggest that synthesis of GlcCer is essential for normal development of A. fumigatus and A. nidulans.

IT **245329-78-6**
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(disruption of the glucosylceramide biosynthetic pathway in Aspergillus)

RN 245329-78-6 CAPLUS

CN Hexadecanamide, N-[(1R,2R)-2-(2,3-dihydro-1,4-benzodioxin-6-yl)-2-hydroxy-1-(1-pyrrolidinylmethyl)ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



REFERENCE COUNT: 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 9 OF 14 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 2001:480708 CAPLUS
DOCUMENT NUMBER: 135:76788
TITLE: Novel amino ceramide-like compounds as glucosyl ceramide (GlcCer) formation inhibitors
INVENTOR(S): Shayman, James A.; Radin, Norman S.
PATENT ASSIGNEE(S): The Regents of the University of Michigan, USA
SOURCE: U.S., 31 pp., Cont.-in-part of U.S. 6,051,598.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 4
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 6255336	B1	20010703	US 1999-350768	19990709
US 5916911	A	19990629	US 1996-708574	19960905
US 5945442	A	19990831	US 1997-883217	19970626
US 5952370	A	19990914	US 1997-882772	19970626
US 6040332	A	20000321	US 1997-882773	19970626

US 6030995	A	20000229	US 1998-182161	19981029
BR 2000012318	A	20020528	BR 2000-12318	20000707
US 2001041735	A1	20011115	US 2001-870870	20010531
US 6569889	B2	20030527		
US 2003073680	A1	20030417	US 2002-134315	20020429

PRIORITY APPLN. INFO.:
US 1995-4047P P 19950920
US 1996-708574 A3 19960905
US 1997-883218 A2 19970626
US 1999-350768 A 19990709
WO 2000-US18935 W 20000707
US 2001-870870 A2 20010531

OTHER SOURCE(S): MARPAT 135:76788

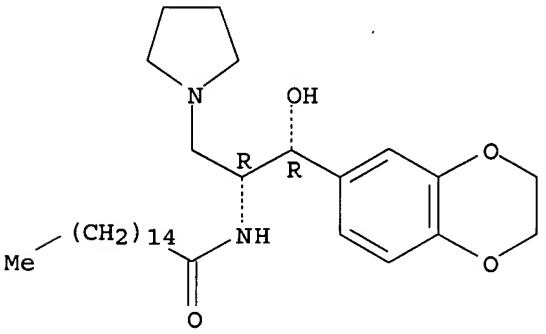
AB The title compds. R1CH(OH)CH(CH2R3)NHCOR2 [I; R1 = (un)substituted Ph, C7-14 alkyl or alkenyl with a double bond next to the kernel of the structure; R2 = (un)satd. (un)substituted alkyl residue of fatty acid; R3 = morpholino, pyrrolidino, piperidino, etc.] which inhibit glucosyl ceramide (GlcCer) formation by inhibiting the enzyme GlcCer synthase, thereby lowering the level of glycosphingolipids, were prepd. E.g., a 3-step synthesis of D-threo-I [R1 = 3',4'-ethylenedioxyphenyl; R2 = C15H31; R3 = pyrrolidino] was presented. Biol.data for compds. I were given. The compds. I have improved GlcCer synthase inhibition activity and are therefore highly useful in therapeutic methods for treating various conditions and diseases assocd. with altered glycosphingolipid levels.

IT **245329-78-6P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(amino ceramide-like compds. as glucosyl ceramide (GlcCer) formation inhibitors)

RN 245329-78-6 CAPLUS

CN Hexadecanamide, N-[(1R,2R)-2-(2,3-dihydro-1,4-benzodioxin-6-yl)-2-hydroxy-1-(1-pyrrolidinylmethyl)ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



REFERENCE COUNT: 50 THERE ARE 50 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 10 OF 14 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER:	2001:50636 CAPLUS
DOCUMENT NUMBER:	134:115797
TITLE:	Synthesis and GlcCer synthase inhibition of amino ceramide-like compounds
INVENTOR(S):	Shayman, James A.; Radin, Norman S.
PATENT ASSIGNEE(S):	Regents of the University of Michigan, USA
SOURCE:	PCT Int. Appl., 62 pp. CODEN: PIXXD2

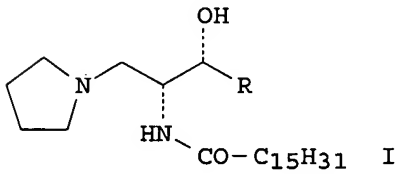
09/288,556

DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 4
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001004108	A1	20010118	WO 2000-US18935	20000707
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
EP 1196406	A1	20020417	EP 2000-945332	20000707
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
BR 2000012318	A	20020528	BR 2000-12318	20000707
JP 2003521479	T2	20030715	JP 2001-509718	20000707

PRIORITY APPLN. INFO.: US 1999-350678 A1 19990709
US 1999-350768 A 19990709
WO 2000-US18935 W 20000707

OTHER SOURCE(S): MARPAT 134:115797
GI



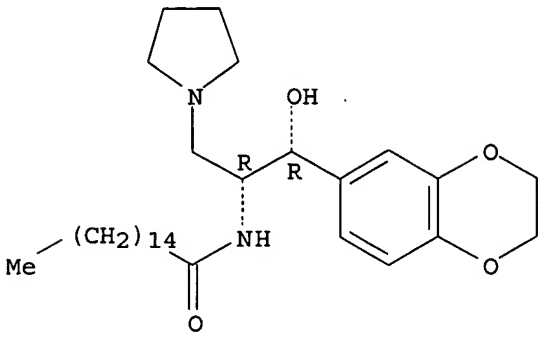
I

AB Synthesis of amino ceramide-like compds. (I) (R = 3,4-ethylenedioxyphenyl, 4-hydroxyphenyl) are disclosed which inhibit glucosyl ceramide (GlcCer) formation by inhibiting the enzyme GlcCer synthase, thereby lowering the level of glycosphingolipids. Thus, I (R = 4-HOC6H4) (II) is prepd. from 4-hydroxyacetophenone by hydroxy protection with benzyl bromide followed by bromination of acetyl, amination of bromide, amidation with palmitoyl chloride, condensation with formaldehyde and pyrrolidine, ketone redn., debenzylation and resoln. with chiral chromatog. II shows an IC50 of 0.5 in GlcCer synthase inhibition assay. The compds. of the present invention have improved GlcCer synthase inhibition activity and are therefore highly useful in therapeutic methods for treating various conditions and diseases assocd. with altered glycosphingolipid levels.

IT **245329-78-6P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(synthesis and GlcCer synthase inhibition of amino ceramide-like compds.)

RN 245329-78-6 CAPLUS
CN Hexadecanamide, N-[(1R,2R)-2-(2,3-dihydro-1,4-benzodioxin-6-yl)-2-hydroxy-1-(1-pyrrolidinylmethyl)ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

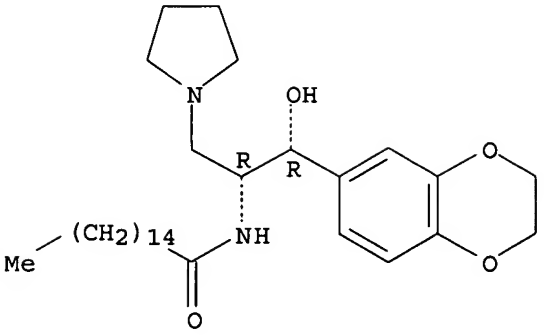
L11 ANSWER 11 OF 14 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 2000:855293 CAPLUS
DOCUMENT NUMBER: 134:256693
TITLE: Use of Sulfobutyl Ether .beta.-Cyclodextrin as a Vehicle for d-threo-1-Phenyl-2-decanoylamino-3-morpholinopropanol-Related Glucosylceramide Synthase Inhibitors
AUTHOR(S): Abe, Akira; Gregory, Susan; Lee, Lihsueh; Shayman, James A.
CORPORATE SOURCE: Nephrology Division, Department of Internal Medicine, University of Michigan Medical School, Ann Arbor, MI, 48109-0676, USA
SOURCE: Analytical Biochemistry (2000), 287(2), 344-347
CODEN: ANBCA2; ISSN: 0003-2697
PUBLISHER: Academic Press
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The sulfobutyl ether linkage of the .beta.-cyclodextrin creates a hydrophilic surface and lipophilic core. The .beta.-cyclodextrin core accommodated each glucosylceramide synthase inhibitor, providing excellent soly. in phosphate-buffered saline. A cyclodextrin-D-threo-1-(3,4-methylenedioxyphenyl)-2-palmitoylamino-3-pyrrolinopropanol (I) complex was easily buffered and could by administered in vivo at concs. suitable for lowering tissue glucosylceramide levels in normal mice. The degree of blobotriaosylceramide depletion in kidneys of the .alpha.-galactosidase A knockout mice was greated when I was complex with sulfobutyl .beta.-cyclodextrin than when liposomes were used. (c) 2000 Academic Press.

IT **245329-78-6**
RL: BPR (Biological process); BSU (Biological study, unclassified); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); PROC (Process); USES (Uses)
(.beta.-cyclodextrin sulfobutyl ether as a vehicle for d-threo-1-phenyl-2-decanoylamino-3-morpholinopropanol-related glucosylceramide synthase inhibitors)

RN 245329-78-6 CAPLUS
CN Hexadecanamide, N-[(1R,2R)-2-(2,3-dihydro-1,4-benzodioxin-6-yl)-2-hydroxy-1-(1-pyrrolidinylmethyl)ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



REFERENCE COUNT: 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 12 OF 14 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 2000:414918 CAPLUS
DOCUMENT NUMBER: 133:290942
TITLE: Glycosphingolipid depletion in Fabry disease lymphoblasts with potent inhibitors of glucosylceramide synthase
AUTHOR(S): Abe, Akira; Arend, Lois J.; Lee, Lihsueh; Lingwood, Clifford; Brady, Roscoe O.; Shayman, James A.
CORPORATE SOURCE: Nephrology Division, Department of Internal Medicine and Department of Pathology, University of Michigan Medical Center, Ann Arbor, MI, USA
SOURCE: Kidney International (2000), 57(2), 446-454
CODEN: KDYIA5; ISSN: 0085-2538
PUBLISHER: Blackwell Science, Inc.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Fabry disease is an inherited X-linked disorder resulting in the loss of activity of the lysosomal hydrolase .alpha.-galactosidase A and causing the clin. manifestations of renal failure, cerebral vascular disease, and myocardial infarction. The phenotypic expression of this disorder is manifest by the accumulation of glycosphingolipids contg. .alpha.-galactosyl linkages, most prominently globotriaosylceramide. Based on quant. structure activity studies, the authors recently reported 2 newly designed glucosylceramide synthase inhibitors based on 1-phenyl-2-palmitoylamino-3-pyrrolidino-1-propanol (P4). These inhibitors, 4'-hydroxy-P4 and ethylenedioxy-P4, were evaluated for their ability to deplete globotriaosylceramide and other glucosylceramide-based lipids in Fabry lymphocytes and were compared with N-butyldeoxynojirimycin, another reported glucosylceramide synthase inhibitor. Concns. as low as 10 nmol/L of 4'-hydroxy-P4 and ethylenedioxy-P4 resulted in 70 and 80% depletion, resp., of globotriaosylceramide, with maximal depletion occurring at 3 days of treatment. There was no impairment of cell growth. In contrast, N-butyldeoxynojirimycin only minimally lowered globotriaosylceramide levels, even at concns. as high as 10 .mu.mol/L. Globotriaosylceramide depletion was confirmed by the loss of binding of FITC-conjugated verotoxin B subunit to the lymphoblasts. These findings suggest that selective glucosylceramide synthase inhibitors are highly effective in the depletion of globotriaosylceramide from Fabry cell lines. The authors suggest that these compds. have potential therapeutic utility in the treatment of Fabry disease.

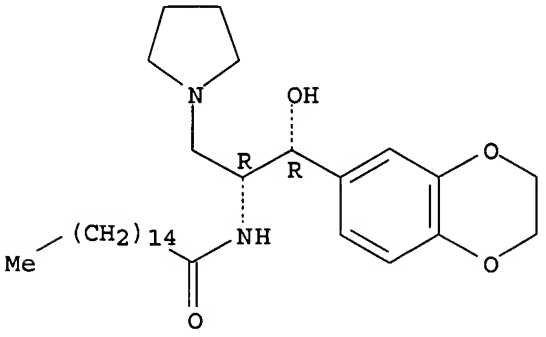
IT **245329-78-6**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(glycosphingolipid depletion in Fabry disease lymphoblasts with glucosylceramide synthase inhibitors)

RN 245329-78-6 CAPLUS

CN Hexadecanamide, N-[(1R,2R)-2-(2,3-dihydro-1,4-benzodioxin-6-yl)-2-hydroxy-1-(1-pyrrolidinylmethyl)ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



REFERENCE COUNT: 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 13 OF 14 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 2000:391547 CAPLUS

DOCUMENT NUMBER: 133:114901

TITLE: Reduction of globotriaosylceramide in Fabry disease mice by substrate deprivation

AUTHOR(S): Abe, Akira; Gregory, Susan; Lee, Lihsueh; Killen, Paul D.; Brady, Roscoe O.; Kulkarni, Ashok; Shayman, James A.

CORPORATE SOURCE: Nephrology Division, Department of Internal Medicine, University of Michigan Medical Center, Ann Arbor, MI, USA

SOURCE: Journal of Clinical Investigation (2000), 105(11), 1563-1571
CODEN: JCINAO; ISSN: 0021-9738

PUBLISHER: American Society for Clinical Investigation

DOCUMENT TYPE: Journal

LANGUAGE: English

AB We used a potent inhibitor of glucosylceramide synthase to test whether substrate deprivation could lower globotriaosylceramide levels in .alpha.-galactosidase A (.alpha.-gal A) knockout mice, a model of Fabry disease. C57BL/6 mice treated twice daily for 3 days with D-threo-1-ethylendioxyphenyl-2-palmitoylamino-3-pyrrolidino-propanol (D-t-EtDO-P4) showed a concn.-dependent decrement in glucosylceramide levels in kidney, liver, and spleen. A single i.p. injection of D-t-EtDO-P4 resulted in a 55% redn. in renal glucosylceramide, consistent with rapid renal glucosylceramide metab. A concn.-dependent decrement in renal and hepatic globotriaosylceramide levels was obsd. in .alpha.-Gal A-males treated for 4 wk with D-t-EtDO-P4. When 8-wk-old .alpha.-Gal A-males were treated for 8 wk with 10 mg/kg twice daily, renal globotriaosylceramide fell to below starting levels, consistent with an .alpha.-galactosidase A-independent salvage pathway for globotriaosylceramide degrdn. Complications obsd. with another glucosylceramide synthase inhibitor, N-butyldeoxynojirimycin, including wt. loss and acellularity of lymphatic organs, were not obsd. with D-t-EtDO-P4. These data suggest that Fabry disease may be amenable to substrate deprivation therapy.

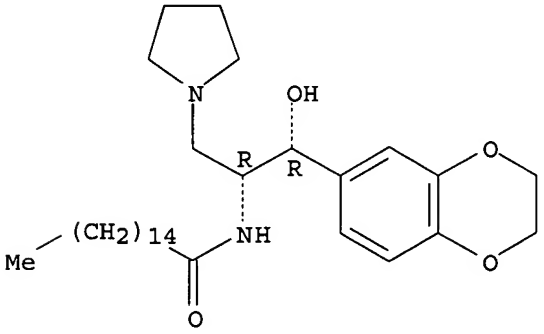
IT **245329-78-6**

RL: ADV (Adverse effect, including toxicity); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(redn. of globotriaosylceramide in Fabry disease mice by substrate deprivation)

RN 245329-78-6 CAPLUS

CN Hexadecanamide, N-[(1R,2R)-2-(2,3-dihydro-1,4-benzodioxin-6-yl)-2-hydroxy-1-(1-pyrrolidinylmethyl)ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



REFERENCE COUNT: 29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 14 OF 14 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1999:466901 CAPLUS

DOCUMENT NUMBER: 131:268809

TITLE: Improved inhibitors of glucosylceramide synthase

AUTHOR(S): Lee, Lihsueh; Abe, Akira; Shayman, James A.

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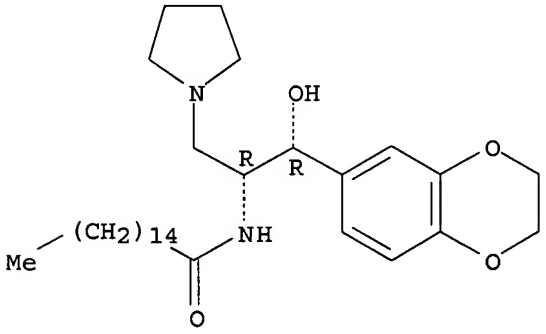
AB Previous work has led to the identification of inhibitors of glucosylceramide synthase, the enzyme catalyzing the first glycosylation step in the synthesis of glucosylceramide-based glycosphingolipids. These inhibitors have two identified sites of action: the inhibition of glucosylceramide synthase, resulting in the depletion of cellular glycosphingolipids, and the inhibition of 1-O-acylceramide synthase, resulting in the elevation of cell ceramide levels. A new series of glucosylceramide synthase inhibitors based on substitutions in the Ph ring of a parent compd., 1-phenyl-2-palmitoylamino-3-pyrrolidino-1-propanol (P4), was made. For substitutions of single functional groups, the potency of these inhibitors in blocking glucosylceramide synthase was primarily dependent upon the hydrophobic and electronic properties of the substituents. An exponential relationship was found between the IC50 of each inhibitor and the sum of derived hydrophobic (.pi.) and electronic (.sigma.) parameters. This relationship demonstrated that substitutions that increased the electron-donating characteristics and decreased the lipophilic characteristics of the homologues enhanced the potency of these compds. in blocking glucosylceramide formation. A novel compd. was subsequently designed and obsd. to be even more active in blocking

glucosylceramide formation. This compd., D-threo-4'-hydroxy-P4, inhibited glucosylceramide synthase at an IC50 of 90 nM. In addn., a series of dioxane substitutions was designed and tested. These included 3',4'-methylenedioxyphenyl-,3',4'-ethylenedioxyphenyl-, and 3',4'-trimethylenedioxyphenyl-substituted homologues. D-Threo-3',4'-ethylenedioxy-P4-inhibited glucosylceramide synthase was comparably active to the p-hydroxy homolog. 4'-Hydroxy-P4 and ethylenedioxy-P4 blocked glucosylceramide synthase activity at concns. that had little effect on 1-O-acylceramide synthase activity. These novel inhibitors resulted in the inhibition of glycosphingolipid synthesis in cultured cells at concns. that did not significantly raise intracellular ceramide levels or inhibit cell growth.

IT **245329-78-6P 245329-83-3P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(improved inhibitors of glucosylceramide synthase)

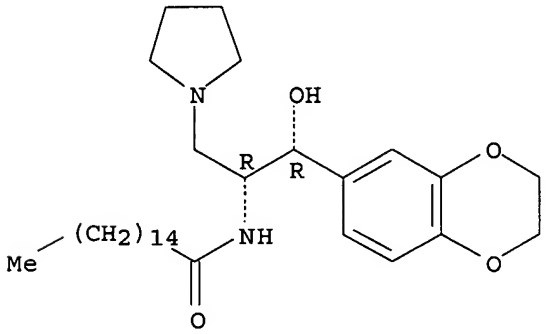
RN 245329-78-6 CAPLUS
CN Hexadecanamide, N-[(1R,2R)-2-(2,3-dihydro-1,4-benzodioxin-6-yl)-2-hydroxy-1-(1-pyrrolidinylmethyl)ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



RN 245329-83-3 CAPLUS
CN Hexadecanamide, N-[(1R,2R)-2-(2,3-dihydro-1,4-benzodioxin-6-yl)-2-hydroxy-1-(1-pyrrolidinylmethyl)ethyl]-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

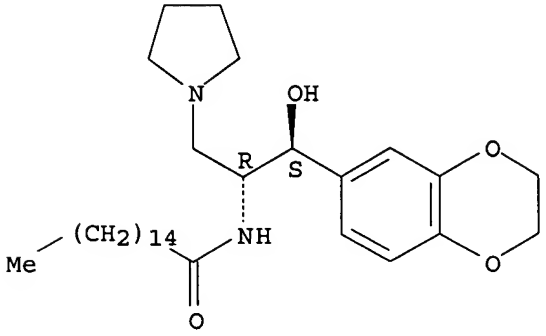


IT **245329-84-4P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(improved inhibitors of glucosylceramide synthase)

RN 245329-84-4 CAPLUS
CN Hexadecanamide, N-[(1R,2S)-2-(2,3-dihydro-1,4-benzodioxin-6-yl)-2-hydroxy-

1-(1-pyrrolidinylmethyl)ethyl]-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



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